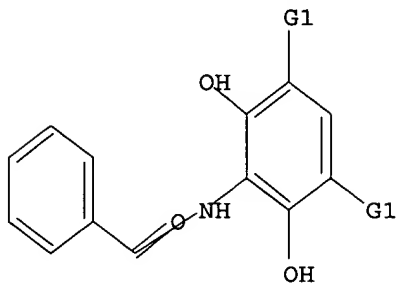
L2 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu

Structure attributes must be viewed using STN Express query preparation.

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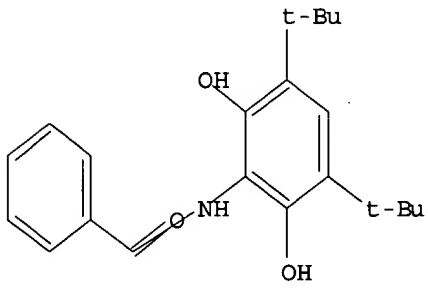
L2 STR



Structure attributes must be viewed using STN Express query preparation.

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FULL SCREEN SEARCH COMPLETED - 2736 TO ITERATE

100.0% PROCESSED 2736 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=> s l2 sss full
FULL SEARCH INITIATED 14:07:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 83 TO ITERATE

100.0% PROCESSED 83 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L4 2 SEA SSS FUL L2

=> file caplus

09/288,556

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	296.70	296.91

FILE 'CAPLUS' ENTERED AT 14:08:10 ON 24 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 24 Jun 2003 VOL 138 ISS 26
FILE LAST UPDATED: 23 Jun 2003 (20030623/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l4
L5 2 L4

=> d l5 1-2 ibib abs hitstr

L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:637509 CAPLUS
DOCUMENT NUMBER: 137:179879
TITLE: N-(3,5-Ditertiarybutyl-2,,6-dihydroxyphenyl)benzamide) pharmaceutical for hyperlipidemia treatment
INVENTOR(S): Tojo, Shinichiro; Nita, Masahiro; Nishimura, Takeski; Shan, Bei
PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Company, Limited, Japan; Tularik Inc.
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002064125	A2	20020822	WO 2002-US4153	20020212
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, IL, IN, IS, KE, KG, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002119958	A1	20020829	US 2001-782535	20010213

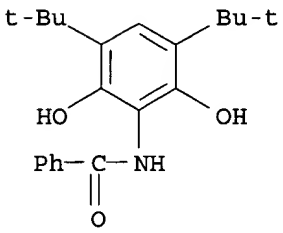
PRIORITY APPLN. INFO.: US 2001-782535 A 20010213

AB The present invention provides a therapeutic agent, e.g., N-(3,5-ditert-butyl-2,6-dihydroxyphenyl)benzamide (I) for the treatment of hyperlipidemia, which has a novel action mechanism and which contains a farnesoid X receptor (FXR) antagonist as an active ingredient, and a screening method of the antagonist. Thus, I was prepd. by the redn. of 2-nitroresorcinol, followed by the reaction of the resulting 2-aminoresorcinol with benzoyl chloride and finally reaction with tert-BuOH. I antagonized the transcription activity-promoting action of FXR, increased the expression of CYP7A gene in the liver and a decrease in the I-BABP gene expression in the ileum.

IT **403793-75-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(ditert-butyl(dihydroxyphenyl)benzamide pharmaceutical for hyperlipidemia treatment)

RN 403793-75-9 CAPLUS

CN Benzamide, N-[3,5-bis(1,1-dimethylethyl)-2,6-dihydroxyphenyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:185060 CAPLUS
DOCUMENT NUMBER: 136:247408
TITLE: Preparation of amides as farnesoid X receptor modulators
INVENTOR(S): Houze, Jonathan; McKendry, Sharon; Gergely, Joshua P.; Xia, Yi; Shan, Bei; Kayser, Frank
PATENT ASSIGNEE(S): Tularik Inc., USA
SOURCE: PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

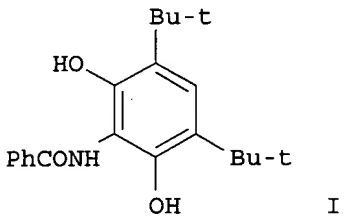
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002020463	A2	20020314	WO 2001-US27239	20010831
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001088623	A5	20020322	AU 2001-88623	20010831
US 2002120137	A1	20020829	US 2001-945293	20010831

PRIORITY APPLN. INFO.: US 2000-230585P P 20000905

US 2000-258092P P 20001222
WO 2001-US27239 W 20010831

OTHER SOURCE(S): MARPAT 136:247408

GI



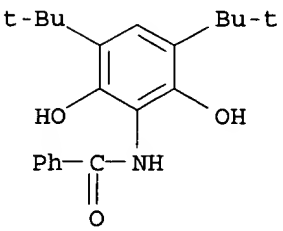
I

AB The present invention provides compds. of formula B-L-A-L1-B1 [A = alkylene, cycloalkylene, arylene, etc.; L, L1 = O, S, CO, CONH, etc.; B, B1 = alkyl, cycloalkyl, aryl, heteroaryl, etc.], pharmaceutical compns. and methods that are useful in modulating the farnesoid X receptor (FXR). As FXR is involved in neg. controlling the expression level of cholesterol 7.alpha.-hydroxylase (cyp7a), the rate-limiting enzyme involved in the oxidative metab. of cholesterol into bile acids, the compds. described herein find utility in treating diseases assocd. with abnormally high or low cholesterol levels. In certain aspects, the FXR modulators (e.g., antagonists) described herein block the neg. feed-back downregulation of cyp7a expression produced by certain cholic acids, the endogenous ligands for FXR. Moreover, as FXR forms heterodimers with the retinoid X receptor (RXR) in some cell types, modulation of the level of FXR activity in cells has a wide range of effects on a variety of biol. processes which are mediated by RXR or other RXR-interacting proteins such as PPAR.gamma. and PPAR.alpha.. The compds. described herein are useful in treating other biol. activities such as obesity, diabetes, lipid assocd. disorders, cancer, inflammatory disorders, disorders involving a disrupted or dysfunctional epidermal barrier, and various other metabolic disorders. Thus, N-(2,6-dihydroxyphenyl)benzamide was reacted with 2-methyl-2-propanol in H3PO4 to give I in 85% yield. The IC50 values of the compds. were 1-30 .mu.M in FXR binding activity evaluation.

IT **403793-75-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amides as farnesoid X receptor modulators)

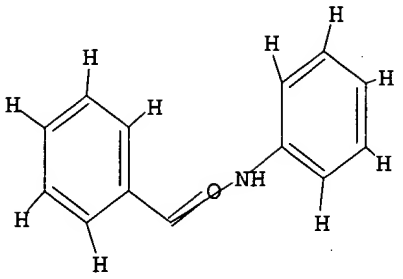
RN 403793-75-9 CAPLUS

CN Benzamide, N-[3,5-bis(1,1-dimethylethyl)-2,6-dihydroxyphenyl]- (9CI) (CA INDEX NAME)



09/288,556

L10 STR



G1 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu

Structure attributes must be viewed using STN Express query preparation.

=> s l10 sss full
FULL SEARCH INITIATED 14:13:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 579487 TO ITERATE

69.0% PROCESSED 400000 ITERATIONS 10 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.04

FULL FILE PROJECTIONS:	ONLINE	**INCOMPLETE**
	BATCH	**COMPLETE**
PROJECTED ITERATIONS:	579487 TO	579487
PROJECTED ANSWERS:	10 TO	25

L11 10 SEA SSS FUL L10

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	148.95	609.69

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.95

FILE 'CAPLUS' ENTERED AT 14:13:19 ON 24 JUN 2003
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FILE COVERS 1907 - 24 Jun 2003 VOL 138 ISS 26
FILE LAST UPDATED: 23 Jun 2003 (20030623/ED)

This file contains CAS Registry Numbers for easy and accurate

substance identification.

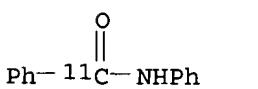
=> s l11
L12 9 L11

=> d l12 1-9 ibib abs hitstr

L12 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2003:247918 CAPLUS
DOCUMENT NUMBER: 138:401472
TITLE: Aryl Triflates and [11C]/(13C)Carbon Monoxide in the Synthesis of 11C-/13C-Amides
AUTHOR(S): Rahman, Obaidur; Kihlberg, Tor; Lngstroem, Bengt
CORPORATE SOURCE: Department of Organic Chemistry, Institute of Chemistry, Uppsala University, Uppsala, S-751 21, Swed.
SOURCE: Journal of Organic Chemistry (2003), 68(9), 3558-3562
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Palladium(0)-mediated carbonylation reactions using aryl triflates, amines, and a low concn. of [11C]carbon monoxide were used in the syntheses of 13 11C-labeled amides. Lithium bromide was used as an additive to facilitate the reaction. The 11C-labeled products were obtained with decay-cor. radiochem. yields in the range of 2-63%. The radiochem. purity of the final products exceeded 98%. As an example, a reaction starting with 1.79 GBq [11C]carbon monoxide gave 0.38 GBq of LC-purified N-isopropyl-4-nitro-[11C]benzamide within 27 min from the start of the carbonylation reaction (54% decay-cor. radiochem. yield). The specific radioactivity of this compd. was 191 GBq/.mu.mol, 35 min after the end of a 10 .mu.Ah bombardment. N-Benzylisoquinoline-1-(13C)carboxamide was prepd. and analyzed by NMR for confirmation of the labeling position. The starting triflates were synthesized from the alcs. and trifluoromethanesulfonic anhydride. The ref. compds. RCONHCH2Ph [R = 3-pyridyl, 1-isoquinolyl] were prepd. from RCO2H and PHCH2NH2. The other nine ref. compds. were synthesized from the acid chlorides and amines. The present report shows that the sometimes more easily obtainable aryl triflates can be a useful alternative to the commonly used aryl halides in palladium(0)-mediated synthesis of 11C/13C-amides.

IT **529493-61-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of labeled amides from aryl triflates and labeled carbon monoxide)
RN 529493-61-6 CAPLUS
CN Benzamide-carbonyl-11C, N-phenyl- (9CI) (CA INDEX NAME)



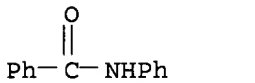
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:174741 CAPLUS
DOCUMENT NUMBER: 137:369813
TITLE: Organoiridium catalyzed hydrogen isotope exchange of benzamide derivatives

AUTHOR(S): Valsborg, Jacob S.; Sorensen, Lone; Foged, Christian
CORPORATE SOURCE: Novo Nordisk A/S, Malov, DK-2760, Den.
SOURCE: Synthesis and Applications of Isotopically Labelled Compounds, Proceedings of the International Symposium, 7th, Dresden, Germany, June 18-22, 2000 (2001), Meeting Date 2000, 72-75. Editor(s): Pleiss, Ulrich; Voges, Rolf. John Wiley & Sons Ltd.: Chichester, UK. CODEN: 69CIJC; ISBN: 0-471-49501-8
DOCUMENT TYPE: Conference
LANGUAGE: English

AB The successful labeling of different benzamide derivs. and acetanilide in the ortho position in the ring using homogeneous catalysis with [Ir(cod)(Cy3P)(Py)]PF6 (Crabtree's catalyst) is described. Crabtree's catalyst has been reported to catalyze exchange of hydrogens exactly four bonds away from the coordinative heteroatom in the substrate. The benzamides are substrates requiring five-membered metallacycle intermediates for hydrogen exchange. The labeling of more complex benzamides with drug-like substituent showed that when the substituent is tetrazole no reaction occurs. This could be due to the presence of the coordinative nitrogen function at the tetrazole which decreases the ability of the iridium complex to participate in reversible interactions with the amide group. A one pot approach can be applied when tritiation of a series of compds. is required.

IT **475203-37-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(organoiridium catalyzed regioselective hydrogen isotope exchange of benzamide derivs.)
RN 475203-37-3 CAPLUS
CN Benzamide, N-phenyl-, labeled with tritium (9CI) (CA INDEX NAME)



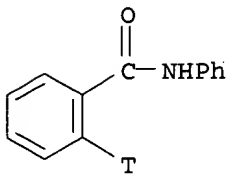
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:151107 CAPLUS
DOCUMENT NUMBER: 134:326254
TITLE: Organoiridium catalyzed hydrogen isotope exchange of benzamide derivatives
AUTHOR(S): Valsborg, Jacob S.; Sorensen, Lone; Foged, Christian
CORPORATE SOURCE: Isotope Chemistry, Novo Nordisk Health Care A/S, Malov, DK-2760, Den.
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (2001), 44(3), 209-214
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:326254

AB Hydrogen-tritium exchange in a series of benzamide derivs. and acetanilide has been investigated using [Ir(cod)(Cy3P)(Py)]PF6 as catalyst. Specific activities of 6-43 Ci/mmol were obtained. Tritium NMR spectroscopy showed that exchange occurred ortho to the amide group.

IT **336625-81-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(organoiridium catalyzed hydrogen isotope exchange of benzamide derivs.)

RN 336625-81-1 CAPLUS
CN Benzamide-2-t, N-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:847267 CAPLUS
DOCUMENT NUMBER: 134:147282
TITLE: Recognition of Amides by New Rigid Calix[4]arene-Based Cavitands
AUTHOR(S): Arduini, Arturo; Secchi, Andrea; Pochini, Andrea
CORPORATE SOURCE: Dipartimento di Chimica Organica e Industriale, Universita di Parma, Parma, I-43100, Italy
SOURCE: Journal of Organic Chemistry (2000), 65(26), 9085-9091
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:147282

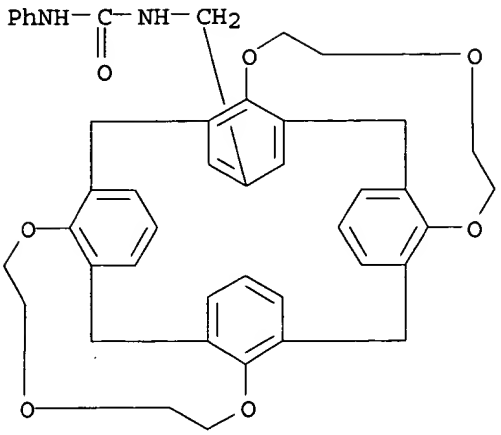
AB The synthesis of new hosts specifically designed for the recognition of amides, characterized by two binding regions: a rigid calix[4]arene cavity and a sidearm, inserted at its rim, able to form strong H bonds, is described. The binding abilities of the new receptors toward amides of general structure R1CONR2R3 were studied in CDCl3 soln. by 1H NMR spectroscopy. When the addnl. binding site is the N-phenylureido group spaced by a methylene unit from the apolar cavity, binding consts. up to 756 M-1 were measured. Neither the two sep. potential binding sites, nor the model host, where the calix[4]arene skeleton is flexible show detectable binding ability toward guests examd. The rigidity of the calix[4]arene apolar cavity is the key control element in detg. the efficiency of these mol. recognition processes. The presence of NH groups in the guest controls the efficiency and selectivity of binding.

IT **323208-56-6**
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(recognition of amides by rigid calix[4]arene-based cavitands)

RN 323208-56-6 CAPLUS
CN Benzamide, N-phenyl-, compd. with N-[(11,12,14,15,27,28,30,31-octahydro-1,25:9,17-dimethano-5H,21H-tetrabenzo[h,k,t,w][1,4,7,13,16,19]hexaoxacyclotetracosin-3-yl)methyl]-N'-phenylurea (1:1) (9CI) (CA INDEX NAME)

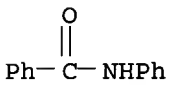
CM 1

CRN 323208-38-4
CMF C44 H44 N2 O7



CM 2

CRN 93-98-1
CMF C13 H11 N O



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:786248 CAPLUS
DOCUMENT NUMBER: 134:115628
TITLE: Solid-State 17O NMR Investigation of the Carbonyl Oxygen Electric-Field-Gradient Tensor and Chemical Shielding Tensor in Amides
AUTHOR(S): Yamada, Kazuhiko; Dong, Shuan; Wu, Gang
CORPORATE SOURCE: Department of Chemistry, Queen's University, Kingston, ON, K7L 3N6, Can.
SOURCE: Journal of the American Chemical Society (2000), 122(47), 11602-11609
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

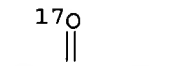
AB A systematic exptl. and theor. study on the carbonyl oxygen elec.-field-gradient (EFG) tensor and chem. shielding (CS) tensor in cryst. amides is presented. Three 17O-labeled secondary amides, R1C[17O]-NHR2, have been synthesized: benzanilide (I), N-methylbenzamide (II), and acetanilide (III). Anal. of 17O magic-angle spinning (MAS) and stationary NMR spectra yields not only the magnitude but also the orientation of the carbonyl 17O EFG and CS tensors. For compds. I-III, the carbonyl 17O quadrupolar coupling const. (QCC) and the span of the chem. shift tensor are found to be in the range of 8.5-8.97 MHz and 560-630 ppm, resp. The largest 17O EFG component lies in the amide plane and is perpendicular to the C:O bond, whereas the smallest component is perpendicular to the N-C:O plane. For the carbonyl 17O CS tensor, the principal component with the largest shielding, .delta.33, is perpendicular to the amide plane, and the tensor component corresponding to the least shielding, .delta.11, is in the amide plane approx.

20.degree. off the direction of the C:O bond. Extensive quantum chem. calcns. using d. functional theory (DFT) have been performed for both isolated and hydrogen-bonded mols. of compds. I-III. The calcd. carbonyl 17O EFG and CS tensors from the latter mol. models are in reasonably good agreement with the exptl. values. In particular, the B3LYP/D95** EFG calcns. overestimate the carbonyl 17O QCC by approx. 0.5 MHz. The B3LYP/D95**/GIAO shielding calcns. yield a linear correlation between the calcd. and exptl. data (slope = 1.125 and R2 = 0.9952). The quantum chem. calcns. indicated that the intermol. C:O.cntdot..cntdot..cntdot.H-N hydrogen-bonding interactions play an important role in detg. the carbonyl oxygen EFG and CS tensors for an amide functional group.

IT **263273-79-6P**, Benzamide-17O, N-phenyl-
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(solid-state oxygen-17 NMR study on carbonyl oxygen elec.-field-gradient tensor and chem. shielding tensor in amides)

RN 263273-79-6 CAPLUS

CN Benzamide-17O, N-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:154708 CAPLUS

DOCUMENT NUMBER: 132:270968

TITLE: Oxygen-17 nuclear magnetic resonance of organic solids

AUTHOR(S): Dong, Shuan; Yamada, Kazuhiko; Wu, Gang

CORPORATE SOURCE: Department of Chemistry, Queen's University Kingston, ON, K7L 3N6, Can.

SOURCE: Zeitschrift fuer Naturforschung, A: Physical Sciences (2000), 55(1/2), 21-28
CODEN: ZNASEI; ISSN: 0932-0784

PUBLISHER: Verlag der Zeitschrift fuer Naturforschung

DOCUMENT TYPE: Journal

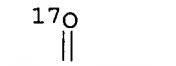
LANGUAGE: English

AB We report solid-state 17O NMR detns. of the oxygen chem. shift (CS) and elec. field gradient (EFG) tensors for a series of 17O-enriched org. compds. contg. various functional groups. In several cases, anal. of the 17O magic-angle-spinning (MAS) and static NMR spectra yields both the magnitude and relative orientations of the 17O CS and EFG tensors. We also demonstrate the feasibility of solid-state 17O NMR as a potentially useful technique for studying mol. structure and hydrogen bonding.

IT **263273-79-6**
RL: PRP (Properties)
(oxygen-17 NMR of org. solids)

RN 263273-79-6 CAPLUS

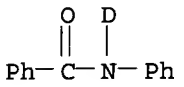
CN Benzamide-17O, N-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

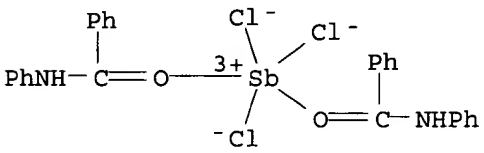
L12 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:496328 CAPLUS
DOCUMENT NUMBER: 129:95215
TITLE: Variable NMR Spin-Lattice Relaxation Times in Secondary Amides: Effect of Ramachandran Angles on Librational Dynamics
AUTHOR(S): Williams, John C.; McDermott, Ann E.
CORPORATE SOURCE: Department of Chemistry, Columbia University, New York, NY, 10027, USA
SOURCE: Journal of Physical Chemistry B (1998), 102(32), 6248-6259
CODEN: JPCBFK; ISSN: 1089-5647
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Deuterium NMR spin-lattice relaxation times (T1Z) of N-deuterated microcryst. secondary amides vary from less than 1 s to more than 500 s at room temp. The main motion effecting relaxation is an out-of-plane libration of the amide, as indicated by temp.-dependent line shapes and anisotropic relaxation spectra. Over 25 amides were measured; they vary with respect to side chain sterics, hydrogen bond lengths, hydrogen bond geometry, and crystal packing. The temp.-dependent deuterium line shape and anisotropic relaxation rates indicate an out-of-plane angular deflection of approx. 10.degree.; the angle is probably similar for the rapidly and slowly relaxing amides, while the apparent time const. for the motion probably varies dramatically. Deuterons in methylene groups on both sides of the amide group for caprylolactam and caprolactam also indicate an out-of-plane libration with relaxation rates somewhat faster than that of the amide deuteron; the angular extent of the distortion is somewhat greater for the flanking .alpha.-deuteron than for the amide deuteron. Carbon relaxation measurements on lauryllactam indicate that the whole mol. librates to a comparable extent. Temp.-dependent relaxation rates for caprylolactam and caprolactam showed non-Arrhenius monotonic increases in the relaxation rates with increasing temp., as expected for libration dynamics; furthermore the quadrupolar relaxation measurements support the assumption that the dominant spectral d. contribution is above the Larmor frequency (i.e. T1Q is longer than T1Z). In aggregate, the data indicate that the motion effecting amide relaxation is a rapid, low-amplitude libration involving the entire mol. Previous work on the librations of amides suggested that these librations are pronounced on the NMR time scale when the substance is near a phase transition; we report here that there is addnl. a relation between the extent of libration and the structure. Comparison of the relaxation times to structures indicates that only amides with flanking alkyl groups on both sides (larger than a Me group) exhibit extensive libration; furthermore predominantly those amides with both flanking dihedral angles, .phi. {C2C1-NC(:O)} and .psi. {N(O:)C-C1'C2'}, near -60.degree. (.apprx..+-.40.degree.) have fast spin-lattice relaxation. No correlation between the deuterium relaxation times and hydrogen bond length nor geometry nor crystal packing was obsd. Variation in the electronic structures of the conjugated amide groups was indirectly probed by measuring the chem. shift anisotropy of the amide carbonyl carbon, the deuterium quadrupolar coupling const., and vibrational frequencies. These parameters did not vary dramatically, indicating that the electronic structure is not strongly variable; the modest variation did not correlate with deuterium relaxation rates. The chem. shift tensor elements were .delta.11 = 91.4 .+-. 5, .delta.22 = 185 .+-. 8, and .delta.33 = 245 .+-. 3 ppm, the quadrupolar coupling const. and its anisotropy were 203 .+-. 10 kHz and 0.15 .+-. 0.02, the NH stretch frequency was 3300 .+-. 42 cm-1, and the carbonyl stretch frequency was 1644 .+-. 25 cm-1. We suggest a model in which the shape of the local potential assocd. with flanking alkyl groups somehow leads to "overdamping" of the amide librational mode.

IT **192878-14-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(effect of Ramachandran angles on librational dynamics in variable NMR spin-lattice relaxation times in secondary amides)
RN 192878-14-1 CAPLUS
CN Benzamide-N-d, N-phenyl- (9CI) (CA INDEX NAME)

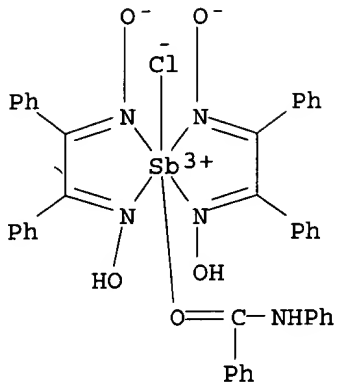


L12 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:24271 CAPLUS
DOCUMENT NUMBER: 128:109905
TITLE: Reactions of some bidentate ligands with antimony trichloride adducts with oxygen donors - I.
AUTHOR(S): Rastogi, M. K.
CORPORATE SOURCE: Department of Chemistry, Hindu College, Delhi, 110 007, India
SOURCE: Asian Journal of Chemistry (1998), 10(1), 150-153
CODEN: AJCHEW; ISSN: 0970-7077
PUBLISHER: Asian Journal of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Stable adducts of antimony trichloride with oxygen donor mols. (urea, formamide, acetamide, DMF, benzamide, acetanilide, benzanilide, and DMSO) on treatment with bidentate ligands (8-hydroxyquinoline, di-Me glyoxime, .alpha.-benzildioxime, .gamma.-benzildioxime and salicylaldoxime) in chloroform in 1:2 molar ratio (except .gamma.-benzildioxime, 1:1 ratio) produce stable complexes by replacing 2 chlorine atoms of the antimony trichloride mol. Some phys. characteristics of the products are reported along with conclusions about their structural mode.

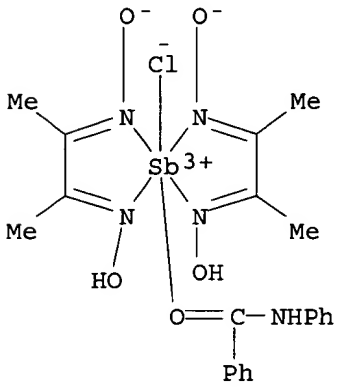
IT **201284-62-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of antimony amide di-Me glyoximato and benzildioximato chloro complexes)
RN 201284-62-0 CAPLUS
CN Antimony, trichlorobis(N-phenylbenzamide-.kappa.O)- (9CI) (CA INDEX NAME)



IT **201284-59-5P 201284-61-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 201284-59-5 CAPLUS
CN Antimony, chlorobis[[diphenylethanedione di(oximato-.kappa.N)](1-)](N-phenylbenzamide-.kappa.O)-, (OC-6-23)- (9CI) (CA INDEX NAME)



RN 201284-61-9 CAPLUS
CN Antimony, bis[[2,3-butanedione di(oximato-.kappa.N)](1-)]chloro(N-phenylbenzamide-.kappa.O)-, (OC-6-23)- (9CI) (CA INDEX NAME)



L12 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:620074 CAPLUS
DOCUMENT NUMBER: 124:131526
TITLE: Positively working resist composition containing carboxamide compound
INVENTOR(S): Oie, Masayuki; Tanaka, Hideyuki; Abe, Nobunori; Misawa, Mari
PATENT ASSIGNEE(S): Nippon Zeon Co, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 23 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07092681	A2	19950407	JP 1993-312672	19931118

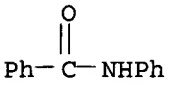
PRIORITY APPLN. INFO.: JP 1993-185472 19930629

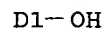
AB The compn. contains (A) an acid-generating compd. by active beam-irradn., (B) a polymer having a structure unit with an acid-unstable group to cleave and be alkali-sol. in the presence of an acid from A, and (C) a carboxamide compd., optionally contg. (D) an alkali-sol. phenolic resin. The compn. is useful for fine processing in manuf. of semiconductor

devices. The compn. showed high sensitivity and gave high-resoln. images with etching resistance and storage stability.

IT **169479-59-8**
RL: TEM (Technical or engineered material use); USES (Uses)
(pos.-working resist compn. contg. carboxamide compd. for manuf. of semiconductor device)

RN 169479-59-8 CAPLUS
CN Benzamide, N-phenyl-, hydroxy deriv. (9CI) (CA INDEX NAME)





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